

Model 2: Growth Curve Fitting

According to A.Tsoularis and our experiment data, we applied Logistic and Gompertz equations to fit the *E.coli* growth curves.

1. The Logistic Growth Curve

The simplest realistic model of *E.coli* population dynamics is the one with exponential growth,

$$\frac{dN}{dt} = rN$$

with solution

$$N(t) = N_0 e^{rt}$$

Where r is the intrinsic growth rate and represents growth rate per capita. To remove unrestricted growth, Verhulst^[2] considered that a stable population would have a saturation level characteristic of the environment. To achieve this the exponential

model was augmented by a multiplicative factor, $1 - \frac{N}{K}$, which represents the

fractional deficiency of the current size from the saturation level, K .

So we have the equation,

$$\frac{dN}{dt} = rN\left(1 - \frac{N}{K}\right)$$

It has solution,

$$N(t) = \frac{KN_0}{(K - N_0)e^{-rt} + N_0}$$

where N_0 is the *E.coli* population size at time $t = 0$,

The three key features of the logistic growth are:

- (i) $\lim_{t \rightarrow \infty} N(t) = K$, the population will ultimately reach its carrying capacity.
- (ii) The relative growth rate, $\frac{1}{N} \frac{dN}{dt}$ declines linearly with increasing population size.
- (iii) The population at the inflection point (where growth rate is maximum), N_{inf} , is exactly half the carrying capacity $N_{inf} = \frac{K}{2}$.

For $r > 0$, the resulting growth curve has a sigmoidal shape and, from (2), is asymptotic to the carrying capacity.

2. The Gompertz Growth Curve

The Gompertz growth curve can be derived from the following form of the logistic equation as a limiting case:

$$\begin{aligned}\frac{dN}{dt} &= \frac{r}{\beta^\gamma} N \left[1 - \left(\frac{N}{K} \right)^\beta \right]^\gamma \\ &= \frac{rN}{K^{\beta\gamma}} \left(\frac{K^\beta - N^\beta}{\beta} \right)^\gamma \\ &= r' N \left(\frac{K^\beta - N^\beta}{\beta} \right)^\gamma\end{aligned}$$

where $r' = \frac{r}{K^{\beta\gamma}}$.

Looking at $\frac{K^\beta - N^\beta}{\beta}$ in the limit as $\beta \rightarrow 0$ we obtain

$$\begin{aligned}\lim_{\beta \rightarrow 0} \frac{K^\beta - N^\beta}{\beta} &= \lim_{\beta \rightarrow 0} \frac{e^{\beta \ln K} - e^{\beta \ln N}}{\beta} \\ &= \lim_{\beta \rightarrow 0} \frac{\sum_{n=0}^{\infty} \frac{(\beta \ln K)^n}{n!} - \sum_{n=0}^{\infty} \frac{(\beta \ln N)^n}{n!}}{\beta} \\ &= \ln \left(\frac{K}{N} \right) + \lim_{\beta \rightarrow 0} \sum_{n=2}^{\infty} \frac{\beta^{n-1}}{n!} \left[(\ln K)^n - (\ln N)^n \right] \\ &= \ln \left(\frac{K}{N} \right)\end{aligned}$$

Similarly, $\lim_{\beta \rightarrow 0} (r') = r, \gamma > 0$

The growth rate modelled by the Gompertz function is given by

$$\frac{dN}{dt} = rN \left[\ln \left(\frac{K}{N} \right) \right]^\gamma$$

For simplicity, we only concern about $\gamma=1$ in the equation

$$\frac{dN}{dt} = rN \left[\ln \left(\frac{K}{N} \right) \right]$$

This is the ordinary Gompertz growth. The solution to it is,

$$N(t) = K \exp \left\{ \ln \left(\frac{N_0}{K} \right) e^{-rt} \right\}$$

The population value at the inflection point, $N_{\text{inf}} = Ke^{-1}$.

We use Curve Fitting Tools (cftool) from Matlab to fit the growth curves of encapsulated and native *E.coli* thus predict the quantitative effect of encapsulation on the growth of bacteria population.

1. *E.coli*@SiO₂:

Fit by Logistic:

Coefficients (with 95% confidence bounds):

$$a = 12.91 \quad (8.869, 16.94)$$

$$b = -0.8453 \quad (-1.136, -0.5549)$$

$$k = 0.5942 \quad (0.4839, 0.7046)$$

Goodness of fit:

SSE: 0.003328

R-square: 0.9906

Adjusted R-square: 0.9875

RMSE: 0.02355

Fitted by Logistic equation:
$$D_L(t) = \frac{0.5942}{1 + e^{12.91 - 0.8453x}}$$

Fit by Gompertz:

General model:

$$f(x) = k \cdot \exp(-\exp(a + b \cdot x))$$

Coefficients (with 95% confidence bounds):

$$a = 6.199 \quad (3.094, 9.303)$$

$$b = -0.4142 \quad (-0.6522, -0.1763)$$

$$k = 0.7271 \quad (0.427, 1.027)$$

Goodness of fit:

SSE: 0.004036

R-square: 0.9886

Adjusted R-square: 0.9848

RMSE: 0.02594

Fitted by Gompertz equation:
$$D_G(t) = 0.7271e^{-e^{6.199 - 0.4142x}}$$

2. Native *E.coli*

Fit by Logistic:

Coefficients (with 95% confidence bounds):

$$a = 1.123 \quad (1.034, 1.213)$$

$$b = -0.2422 \quad (-0.2733, -0.211)$$

$$k = 0.7728 \quad (0.7318, 0.8137)$$

Goodness of fit:

SSE: 0.0008778

R-square: 0.9966
Adjusted R-square: 0.9959
RMSE: 0.009369

Fitted by Logistic equation: $D_L(t) = \frac{0.7728}{1 + e^{1.123 - 0.2422x}}$

Fit by Gompertz:

Coefficients (with 95% confidence bounds):

a = 0.4699 (0.4201, 0.5196)
b = 0.1605 (0.1351, 0.1859)
k = 0.8334 (0.7746, 0.8921)

Goodness of fit:

SSE: 0.000723
R-square: 0.9972
Adjusted R-square: 0.9966
RMSE: 0.008503

Fitted by Gompertz equation: $D_G(t) = 0.8334e^{-e^{0.4699 - 0.1605x}}$

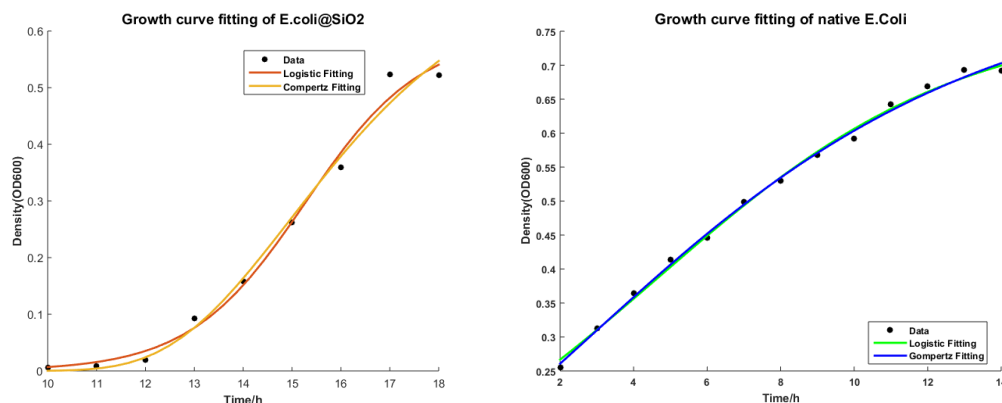


Figure 1 fitting of E.coli growth curves: (left) *E.coli*@SiO₂; (right) native *E.coli*

As shown in the comparison between encapsulated and native groups (Figure 1): the K value for encapsulated bacteria shrinks from 0.7728 in native *E.coli* to 0.5942. Only after 10h of culture do encapsulated group display exponential growth. This confirms the stability of our silicon shell which suppresses the multiply of bacteria.